

Benzoic acid, 4-(aminosulfonyl)-

Other names:	Benzoic acid, 4-(aminosulfonyl)- Benzoic acid, p-sulfamoyl- p-Carboxybenzenesulfonamide p-Sulfamoylbenzoic acid p-Sulfamylbenzoic acid p-Sulfonamidobenzoic acid Benzoic acid p-sulfamide Carzenid Dirnate 4-Carboxybenzenesulfonamide 4-Sulfamoylbenzoic acid 4-Sulfamidobenzoic acid NSC 22976 p-Aminosulfonylbenzoic acid
Inchi:	InChI=1S/C7H7NO4S/c8-13(11,12)6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)(H2,8,11,12)
InchiKey:	UCAGLBKTLXCODC-UHFFFAOYSA-N
Formula:	C7H7NO4S
SMILES:	NS(=O)(=O)c1ccc(C(=O)O)cc1
Mol. weight [g/mol]:	201.20

Physical Properties

Property code	Value	Unit	Source
af	0.8182		Cheméo Relay (1.0)
gf	-556.99	kJ/mol	Joback Method
hf	-578.87	kJ/mol	Cheméo Relay (1.0)
hfus	29.80	kJ/mol	Joback Method
hvap	115.10	kJ/mol	Cheméo Relay (1.0)
ie	9.75	eV	Cheméo Relay (1.0)
log10ws	-2.05		Cheméo Relay (1.0)
logp	0.032		Crippen Method
mcvol	131.240	ml/mol	McGowan Method
pc	6864.13	kPa	Joback Method
tb	598.68	K	Cheméo Relay (1.0)
tc	893.74	K	Cheméo Relay (1.0)
tf	528.28	K	Cheméo Relay (1.0)
vc	0.457	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.53	J/mol×K	657.58	Joback Method
cpg	325.02	J/mol×K	692.73	Joback Method
cpg	332.85	J/mol×K	727.88	Joback Method
cpg	340.02	J/mol×K	763.02	Joback Method
cpg	346.55	J/mol×K	798.17	Joback Method
cpg	352.44	J/mol×K	833.32	Joback Method
cpg	357.69	J/mol×K	868.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C138410&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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